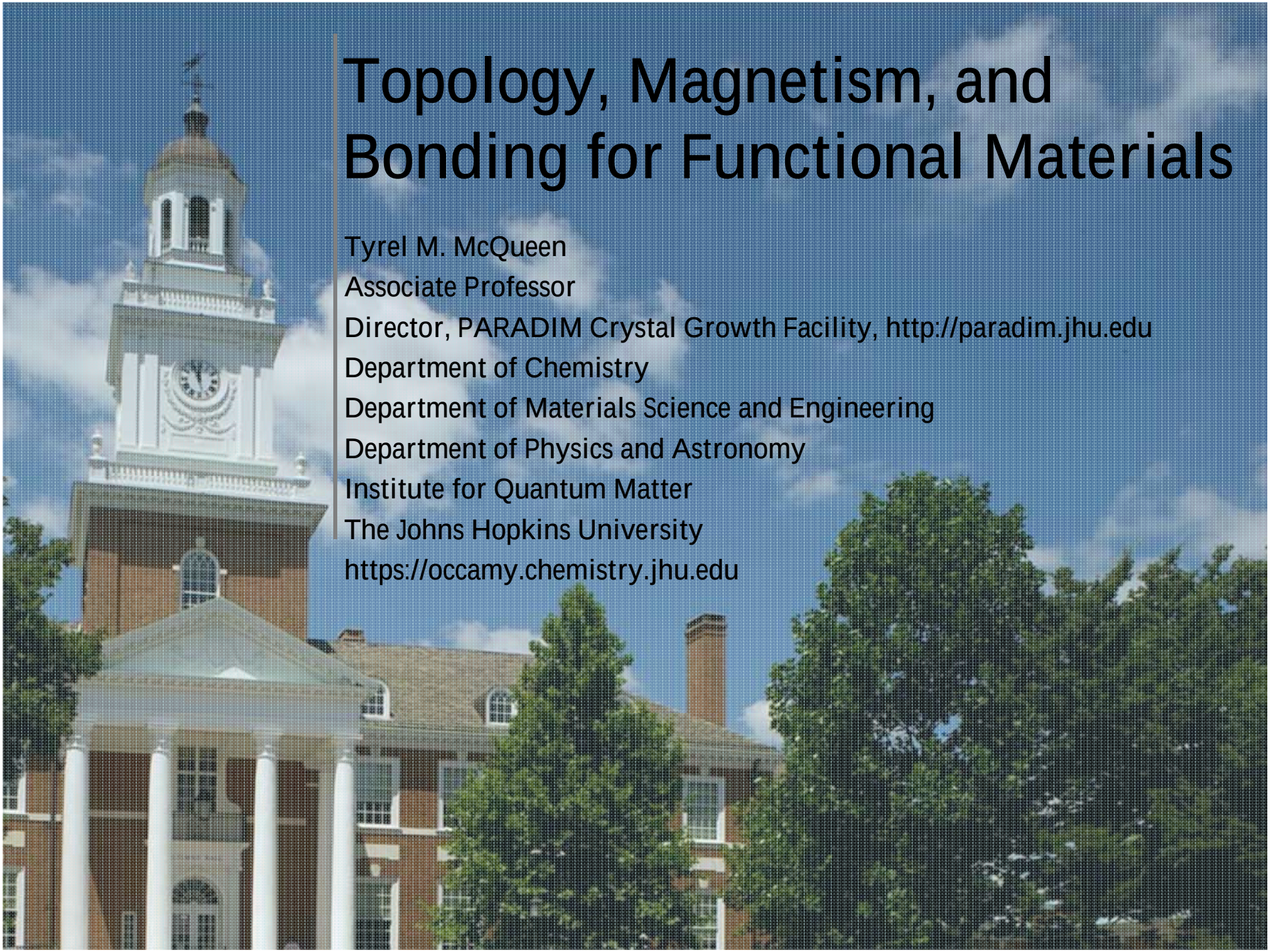
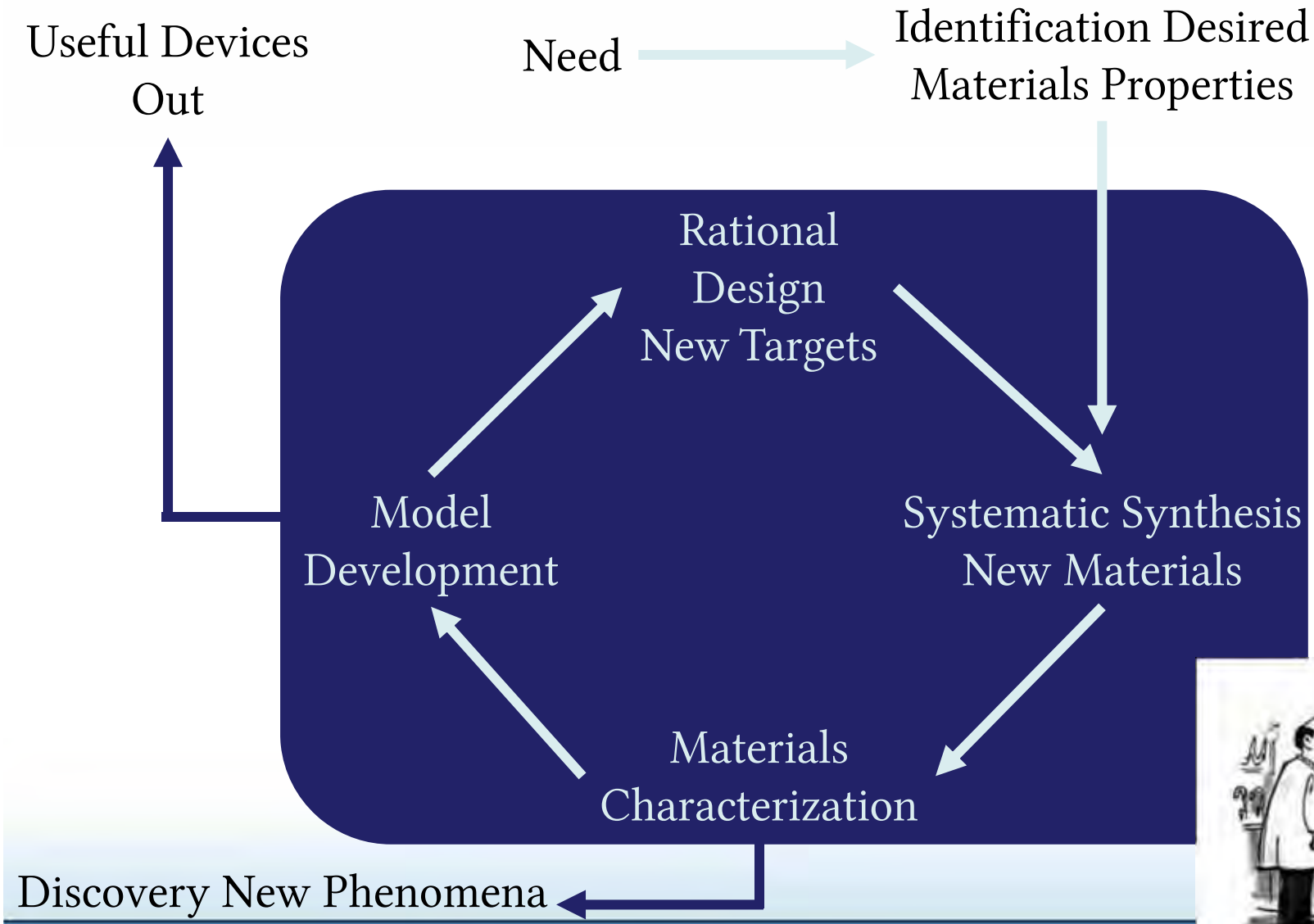


Topology, Magnetism, and Bonding for Functional Materials

Tyrel M. McQueen
Associate Professor
Director, PARADIM Crystal Growth Facility, http://paradim.jhu.edu
Department of Chemistry
Department of Materials Science and Engineering
Department of Physics and Astronomy
Institute for Quantum Matter
The Johns Hopkins University
https://occamy.chemistry.jhu.edu

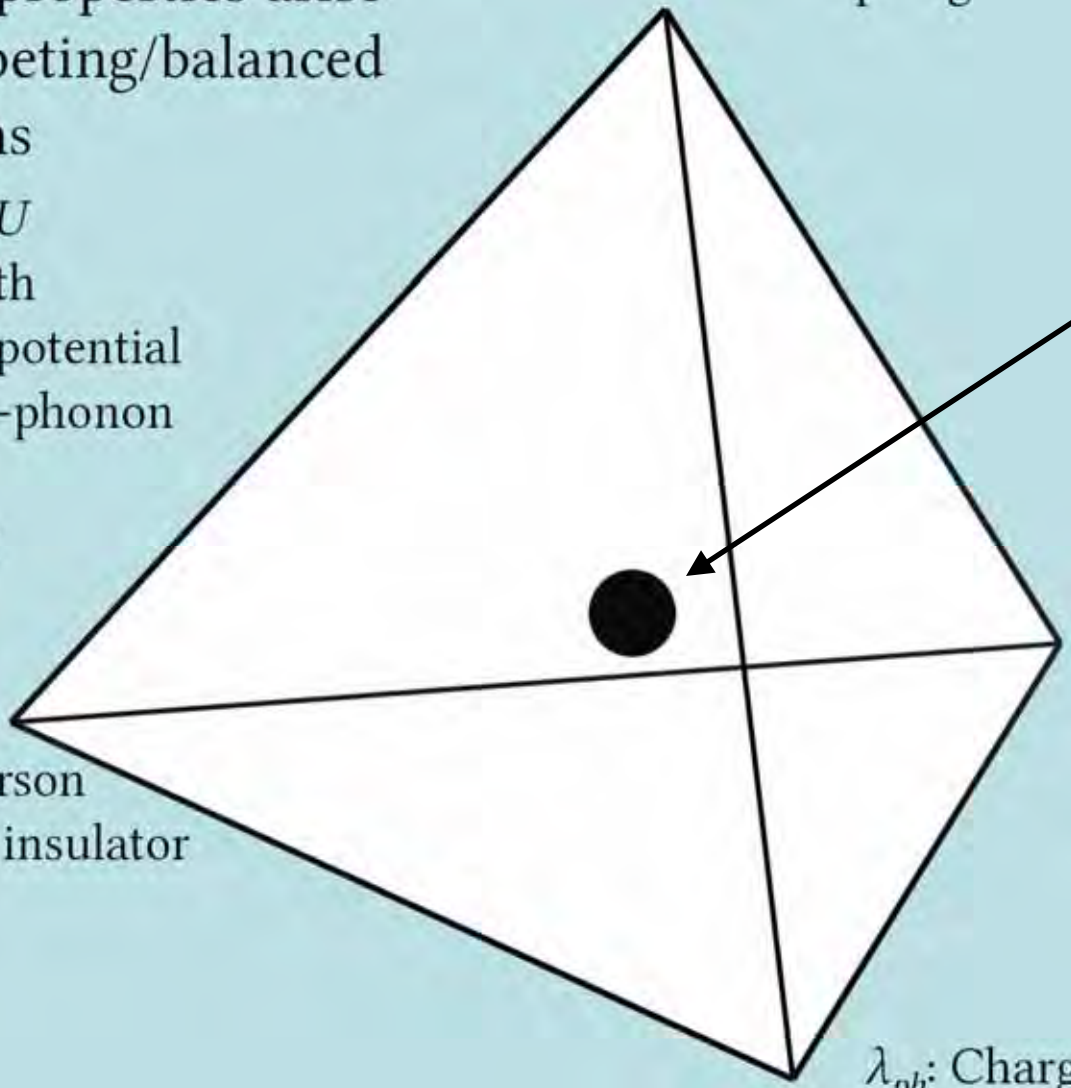
Materials Lifecycle



Energy Scales

Emergent properties arise from competing/balanced interactions

U: Hubbard U
W: Bandwidth
V_0: Random potential
λ_{ph}: Electron-phonon coupling
λ: Spin-orbit coupling



λ/W: Topological band insulator

Band Metal

U/W: Mott-Hubbard insulator

V_0/W: Anderson localization insulator

λ_{ph}: Charge density wave insulator (e.g. Peierls distortion)

Adapted From Tokura

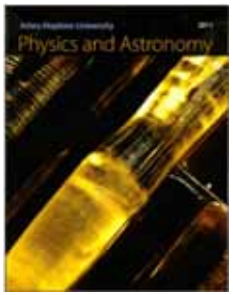
Acknowledgements



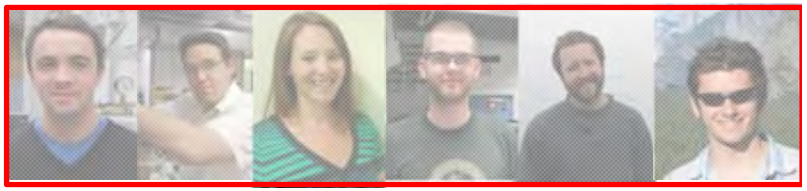


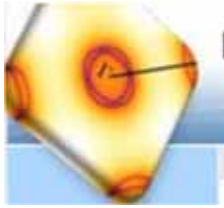











INSTITUTE FOR QUANTUM MATTER

A collaboration between JOHNS HOPKINS UNIVERSITY and PRINCETON UNIVERSITY

Office of Science
U.S. DEPARTMENT OF ENERGY

Funded by the U.S. Department of Energy

NSF

DR
CAREER
PARADIM

PARADIM
PLATFORM FOR THE ACCELERATED REALIZATION, ANALYSIS & DISCOVERY OF INTERFACE MATERIALS

RESEARCH CORPORATION for SCIENCE ADVANCEMENT
A foundation dedicated to science since 1912

the David & Lucile Packard FOUNDATION

ALFRED P. SLOAN FOUNDATION 1934

ACS PRF

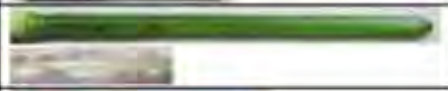
JOHNS HOPKINS UNIVERSITY

https://occamy.chemistry.jhu.edu

Collaborators

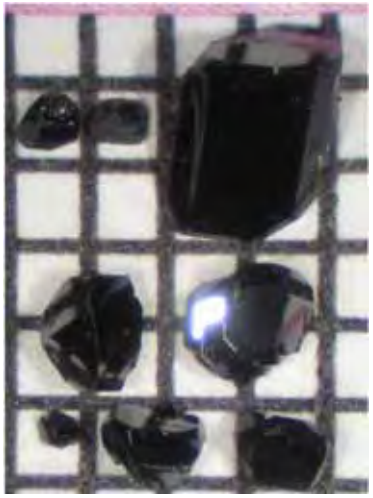
- Dr. T. Birol (Rutgers)
- Dr. P.D.C. King (St. Andrews)
- Dr. Y.F. Nie (Cornell)
- Dr. M. Uchida (Cornell)
- Prof. C.J. Fennie (Cornell)
- Prof. K.M. Shen (Cornell)
- Prof. P. Nikolic (GWU)
- Prof. A. Turner (JHU)
- Prof. C. Broholm (JHU)
- Prof. N.P. Armitage (JHU)
- All collaborators on other projects

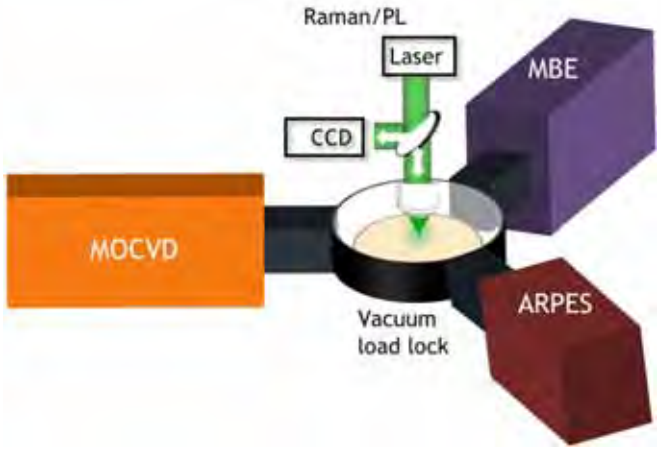
IQM Crystal Growth Successes

Compound	Science	Image	Papers
SmB_6 and LaB_6	Topological Kondo Insulator		1,2
$Pr_2Zr_2O_7$ and $La_2Zr_2O_7$	Quantum Spin Ice		3,4
$SrHo_2O_4$	Frustrated Ladders		5
Bi_2Te_2Se	Topological Insulator		coming
Cd_3As_2	Dirac Semimetal		coming
CeNiSn	Kondo Insulator		coming
$FeSc_2S_4$	Spin-orbital liquid		coming
$CoNb_2O_6$	Critical Ising Chain		6,7
$NiNb_2O_6$	Spin chain		coming
V_2O_3	Mott Insulator		coming
$(V_{1-x}Cr_x)_2O_3$	Spin-orbital insulator		coming
Dy2Ti2O7	Classical spin ice		coming
$MgCr_2O_4$	Spinel Classical spins		8
$SrCr_2O_4$	Triangular lattice		9
$TbMnO_3$	Multi-ferroic		10, 11
TiO_2	Optical		coming
Tl_5Te_3	Topological Superconductor		12
$Yb_2Ti_2O_7$	Quantum Spin Ice		13
YbB_6	Kondo Insulator		coming

Not an exhaustive list!

Materials by Design Gets Serious!





ACTIVE SUBSTRATE + THIN FILM

New $25 Million NSF "Platform" on Interface Materials —*by Design!*

Director: Darrell Schlom (Cornell)

PARADIM

PLATFORM FOR THE ACCELERATED REALIZATION, ANALYSIS & DISCOVERY OF INTERFACE MATERIALS

New Chemistry
New Physics
New Materials Science

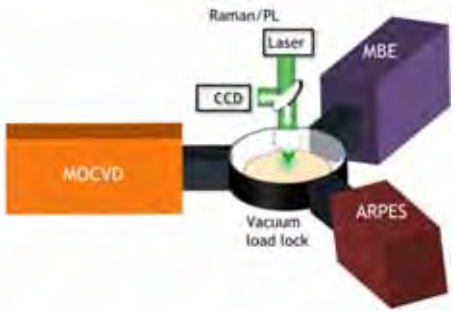
PARADIM: Unique Capabilities

High-pressure (supercritical fluid) floating-zone growth

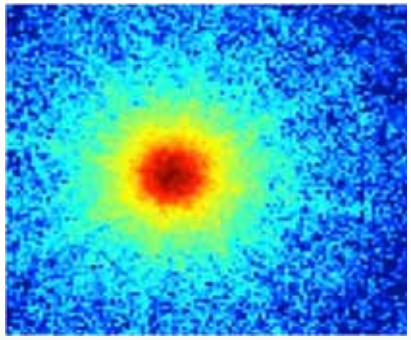
Mass spectrometry and structure *during* bulk crystal growth

Integrated MOCVD + MBE + ARPES

High sensitivity, high dynamic range pixel array detector for quantitative mapping of ***E*** and ***B*** fields with sub-nm resolution



Stable cryo-stages for STEM and STEM-EELS at 20 K and 80-1200 K



Available to the community via proposals

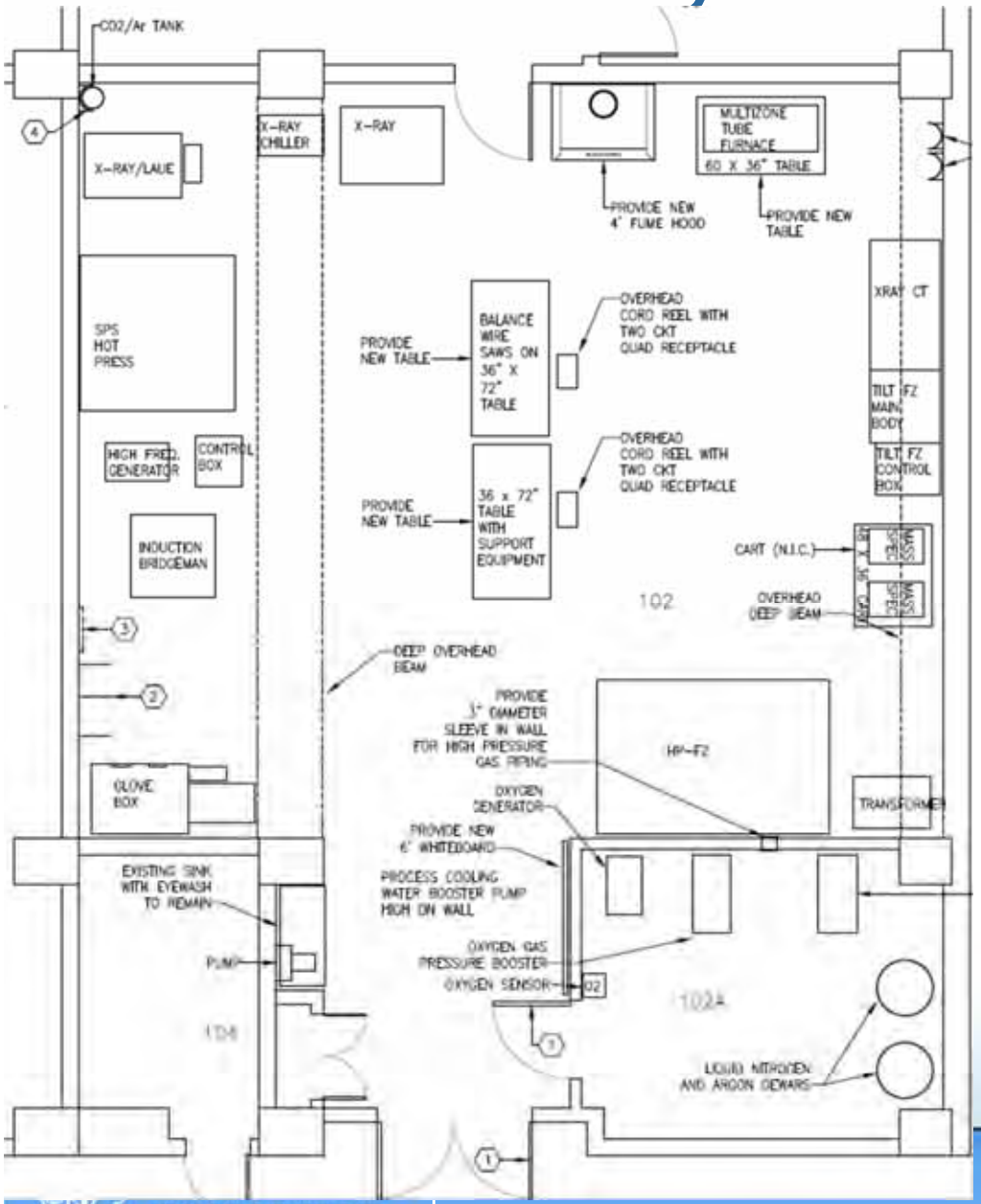
http://paradim.cornell.edu

Summer Schools to build a community of practitioners

Crystal Growth and Design, July 10th-15th, 2016

Intro to Density Functional Theory for Experimentalists, July 25th-29th, 2016

Bulk Crystal Growth at JHU



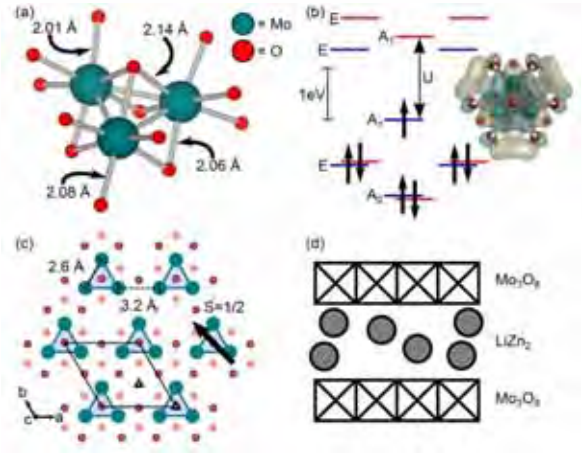
INSTITUTE FOR QUANTUM MATTER

A collaboration between JOHNS HOPKINS UNIVERSITY and PRINCETON UNIVERSITY

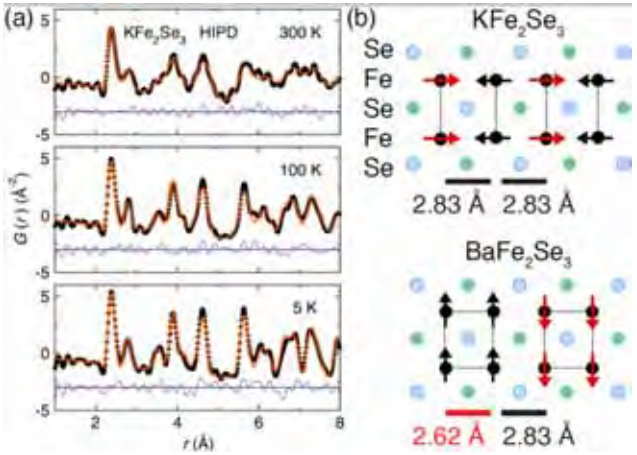
- Leverage existing capabilities within IQM, while providing IQM staff proposal-free access to PARADIM facilities
- Focus is on supercritical fluid and in situ monitoring
  - Complements existing US efforts to expand capabilities in pressure
- Summer schools for building community
- International and industrial partnerships welcome

UNIVERSITY

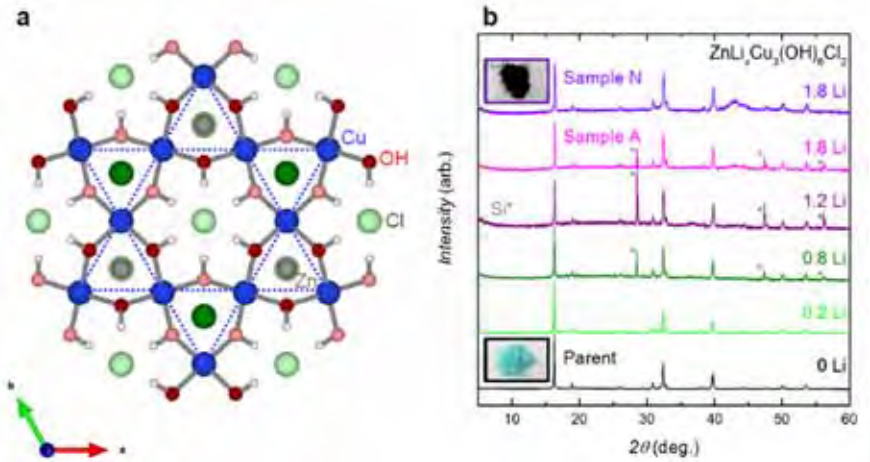
McQueen Laboratory: Research Themes



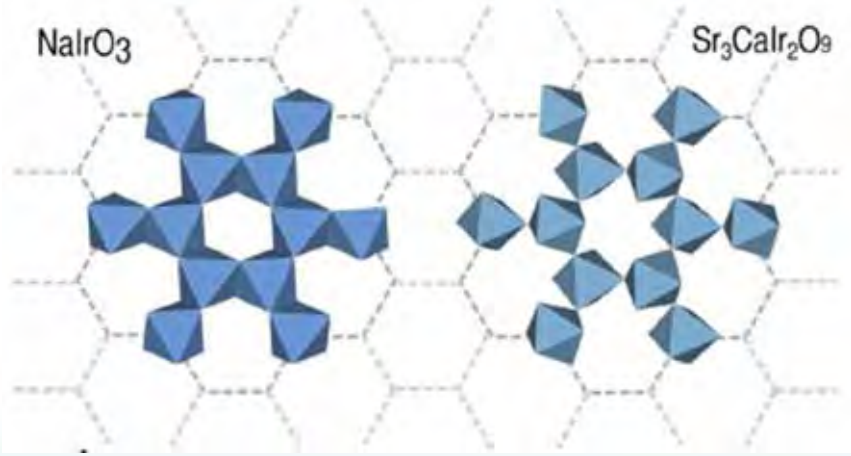
e.g.: J.P. Sheckelton, et al. *Nat. Mater.* **11**, 493-496 (2012)
M. Mourigal, et al. *Phys. Rev. Lett.* **112**, 027202 (2014)



e.g.: J.M. Caron, et al. *Phys. Rev. B (Rapid)* **85**, 180405 (2012)
M. Mourigal, et al. *Phys. Rev. Lett.* **115**, 047401 (2015)



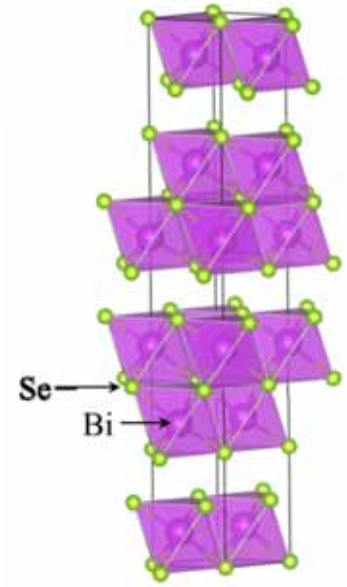
e.g.: Z.A. Kelly, et al. Submitted (2016)



e.g.: D.C. Wallace, et al. *Dalton Transactions* **44**, 20344-51 (2015)

Enough of the advertising… onto the science

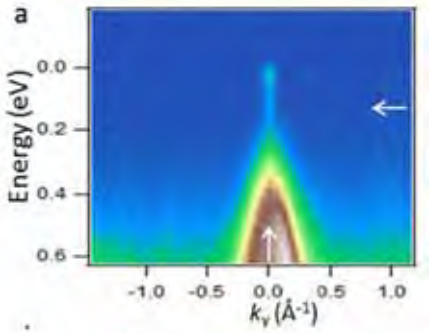
TIs and TCIs

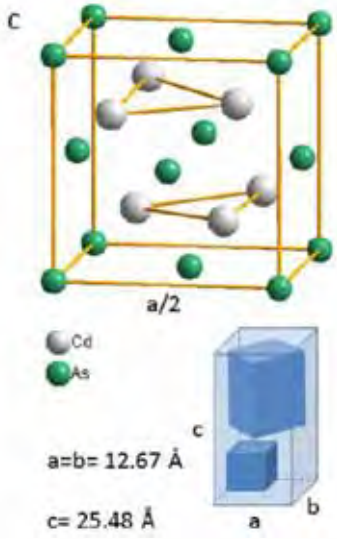


Bi_2Se_3

$Bi_{1-x}Sb_x$
$[Bi]_x[Bi_2(Se/Te)_3]_y$
$TlBi(Se/Te)_2$
$[GeTe]_x[Bi_2Te_3]_y$
*$Bi_{14}Rh_3I_9$
*(Hg/Cd)Te
**(Sn/In)Te

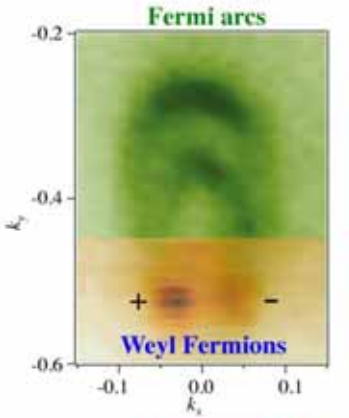
3D Dirac Semimetal

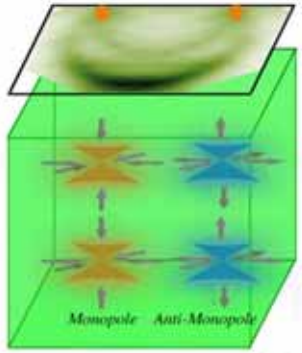




Cd_3As_2
Na_3Bi

Weyl Semimetals

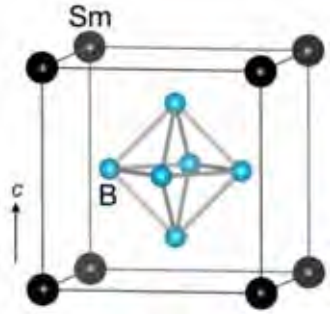


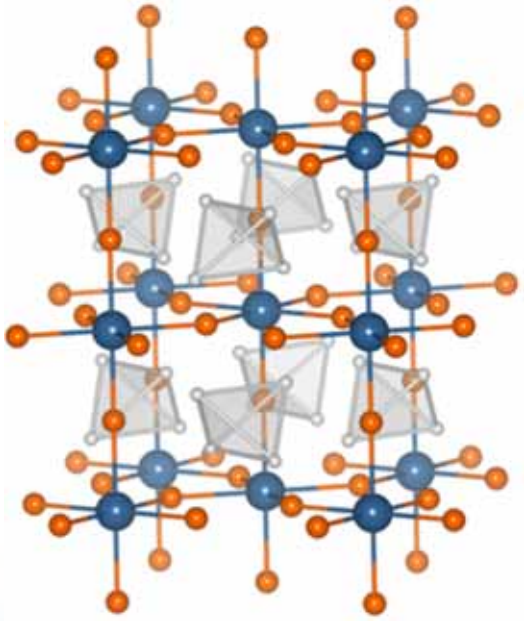


Weyl Fermion Crystal

TaAs
$YbMnBi_2$

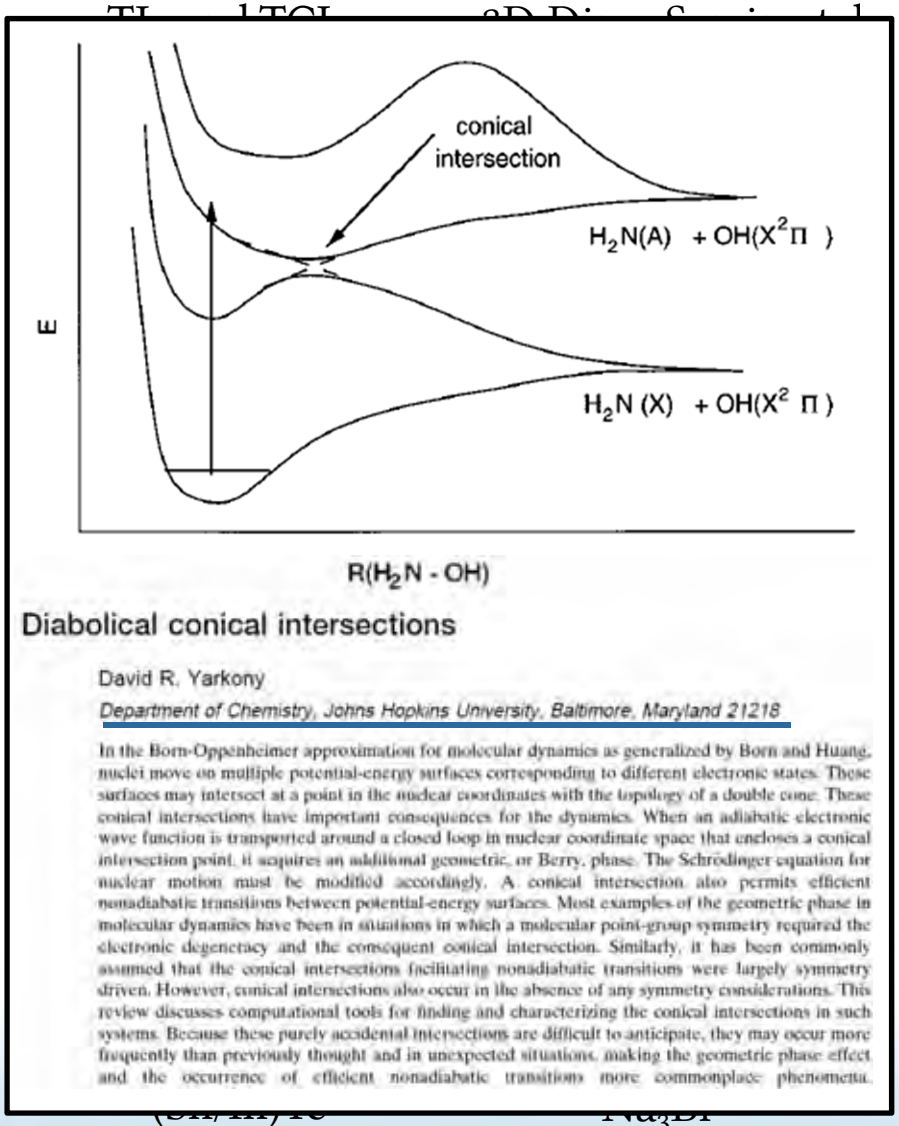
Dirac States with Interactions





Iridates, SmB_6
$[Tl_4]TlTe_3$

Enough of the advertising... onto the science



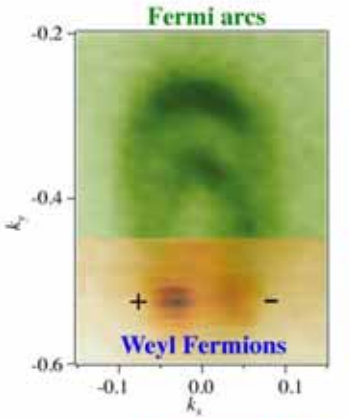
Diabolical conical intersections

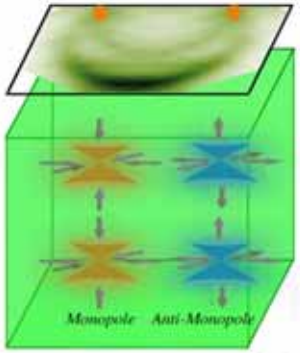
David R. Yarkony

Department of Chemistry, Johns Hopkins University, Baltimore, Maryland 21218

In the Born-Oppenheimer approximation for molecular dynamics as generalized by Born and Huang, nuclei move on multiple potential-energy surfaces corresponding to different electronic states. These surfaces may intersect at a point in the nuclear coordinates with the topology of a double cone. These conical intersections have important consequences for the dynamics. When an adiabatic electronic wave function is transported around a closed loop in nuclear coordinate space that encloses a conical intersection point, it acquires an additional geometric, or Berry, phase. The Schrödinger equation for nuclear motion must be modified accordingly. A conical intersection also permits efficient nonadiabatic transitions between potential-energy surfaces. Most examples of the geometric phase in molecular dynamics have been in situations in which a molecular point-group symmetry required the electronic degeneracy and the consequent conical intersection. Similarly, it has been commonly assumed that the conical intersections facilitating nonadiabatic transitions were largely symmetry driven. However, conical intersections also occur in the absence of any symmetry considerations. This review discusses computational tools for finding and characterizing the conical intersections in such systems. Because these purely accidental intersections are difficult to anticipate, they may occur more frequently than previously thought and in unexpected situations, making the geometric phase effect and the occurrence of efficient nonadiabatic transitions more commonplace phenomena.

Weyl Semimetals

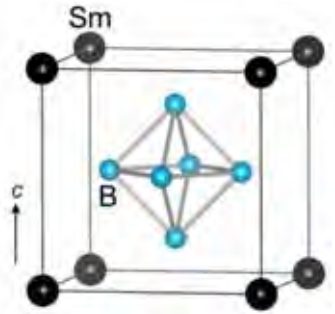


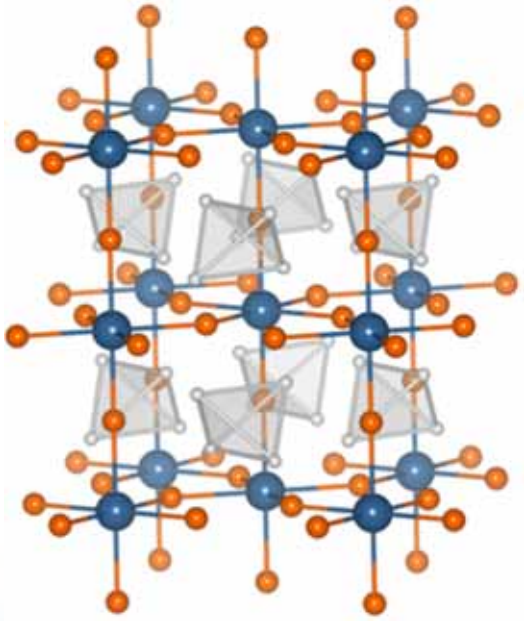


Weyl Fermion Crystal

TaAs
$YbMnBi_2$

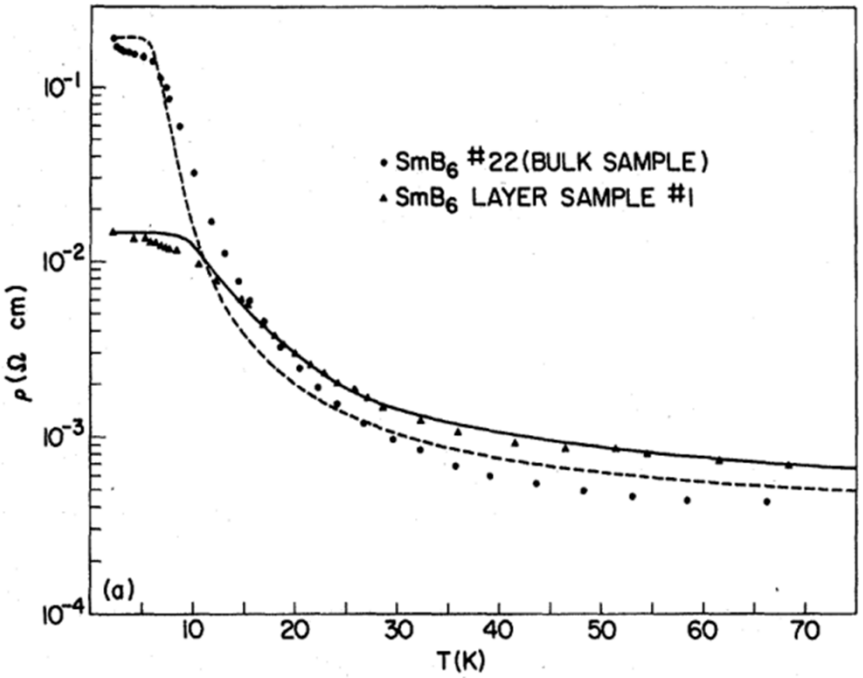
Dirac States with Interactions

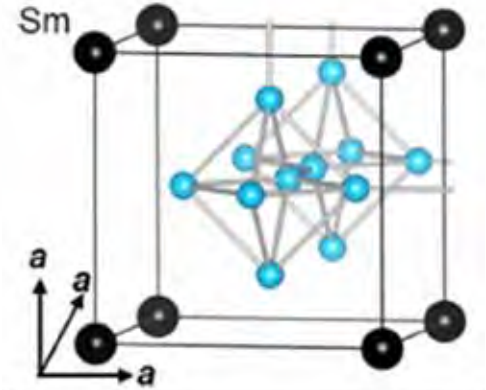


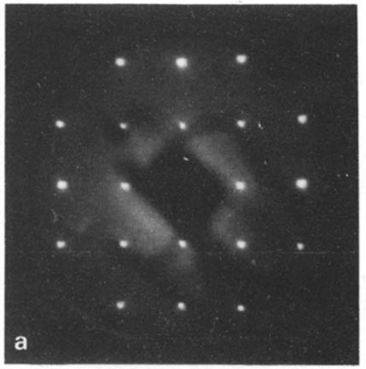


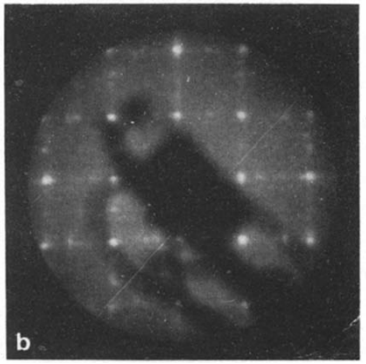
Iridates, SmB_6
$[Tl_4]TlTe_3$

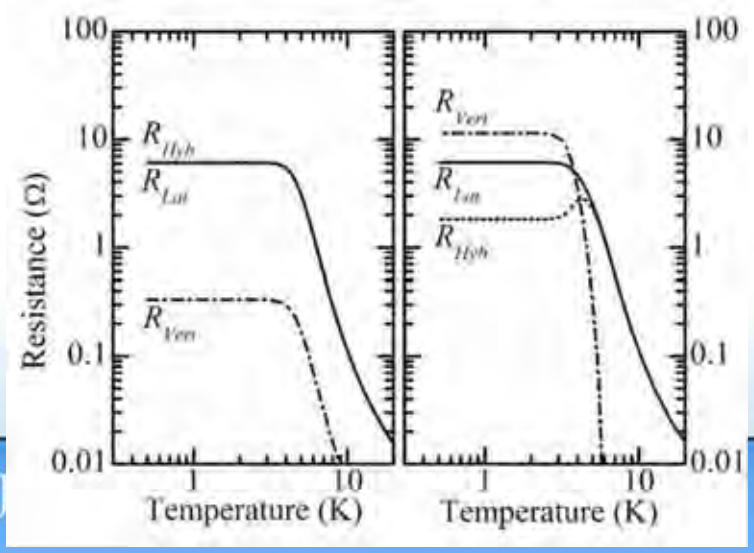
SmB_6: A Topological Insulator?

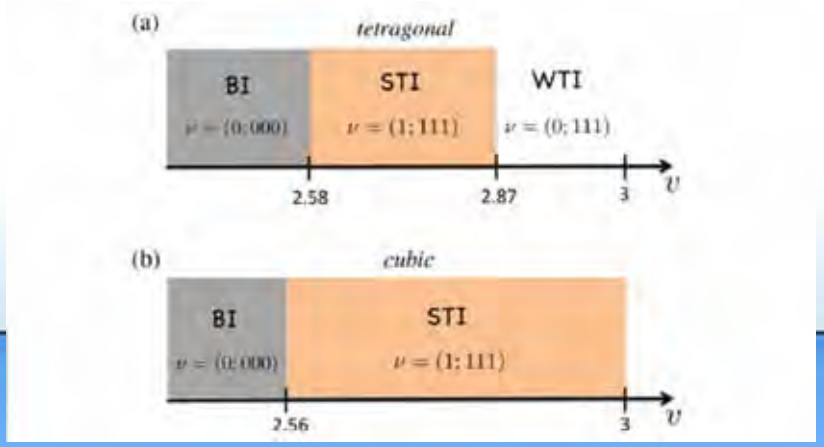




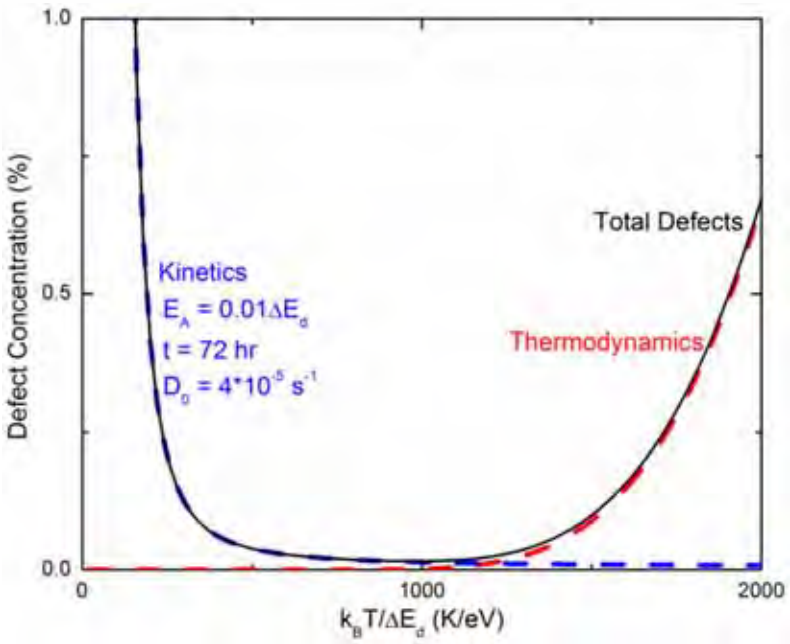


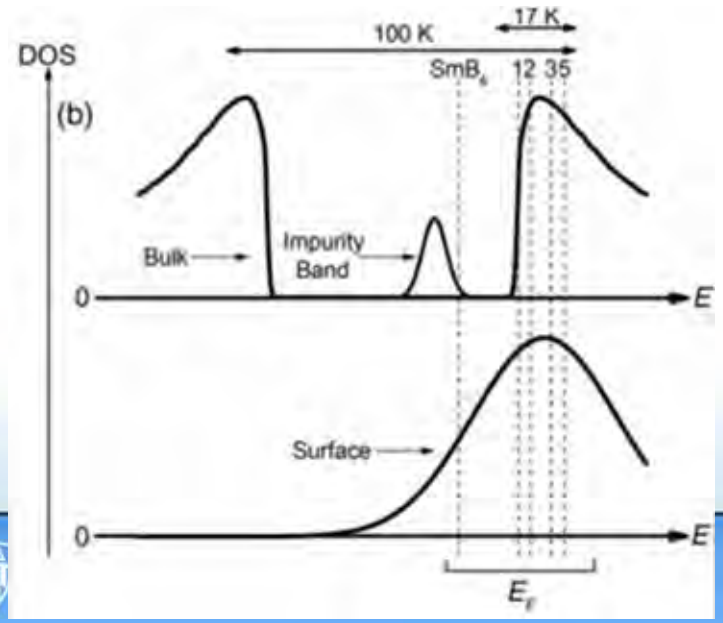




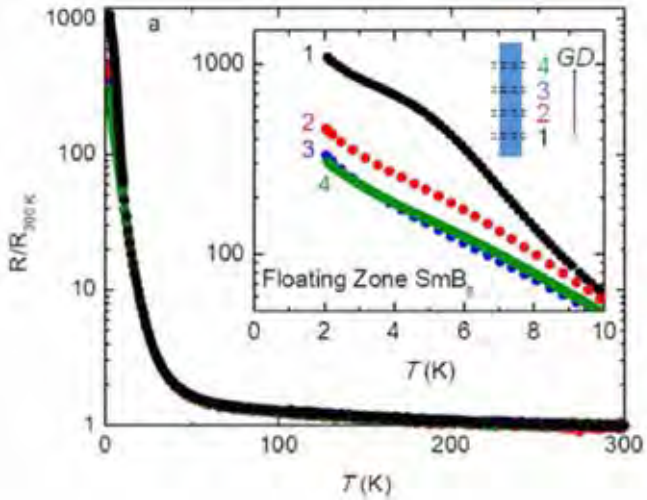


Defects Rule, Physics Drools

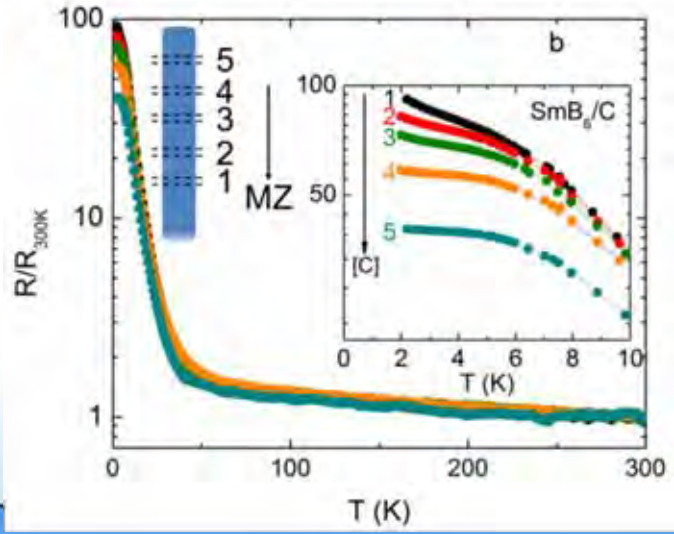




Dope holes via Sm vacancies

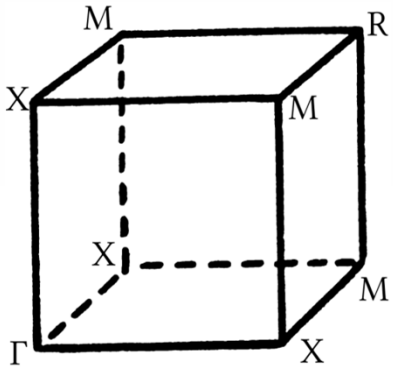


Dope electrons via C for B

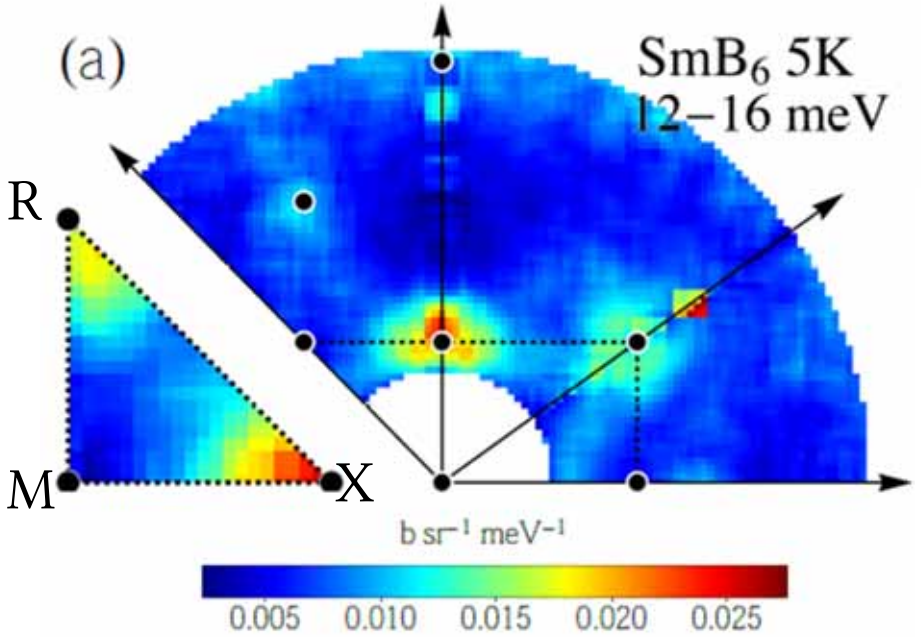


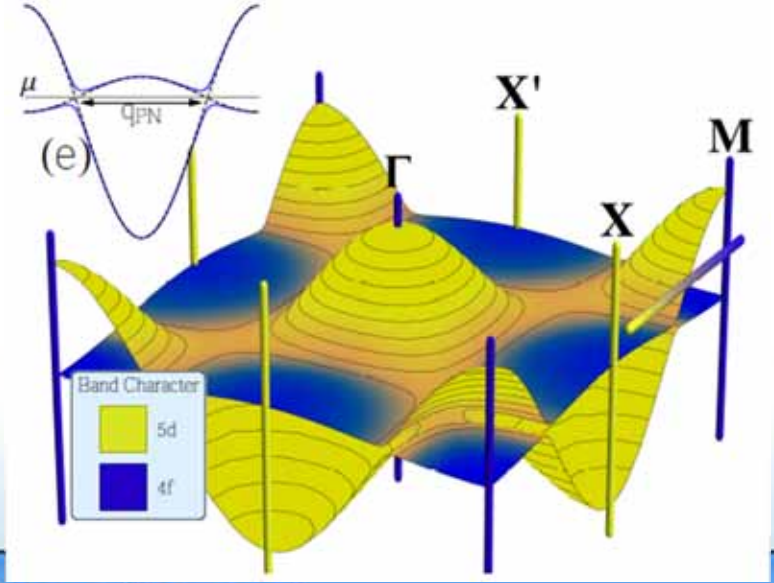
W.A. Phelan, et al. *Phys. Rev. X* 4, 031012 (2014)
W.A. Phelan, et al. *Sci. Rep.* 6, 20860 (2016)

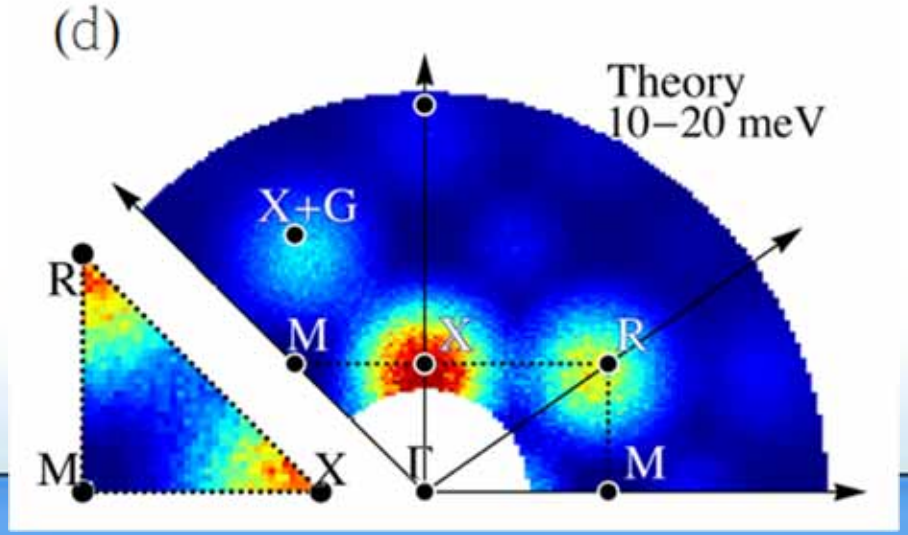
SmB_6: Probably a Strong 3D TI



Product of parities at these 8 points determines topological character







W.T. Fuhrman, et al. *Phys. Rev. Lett.* **114**, 036401 (2015)

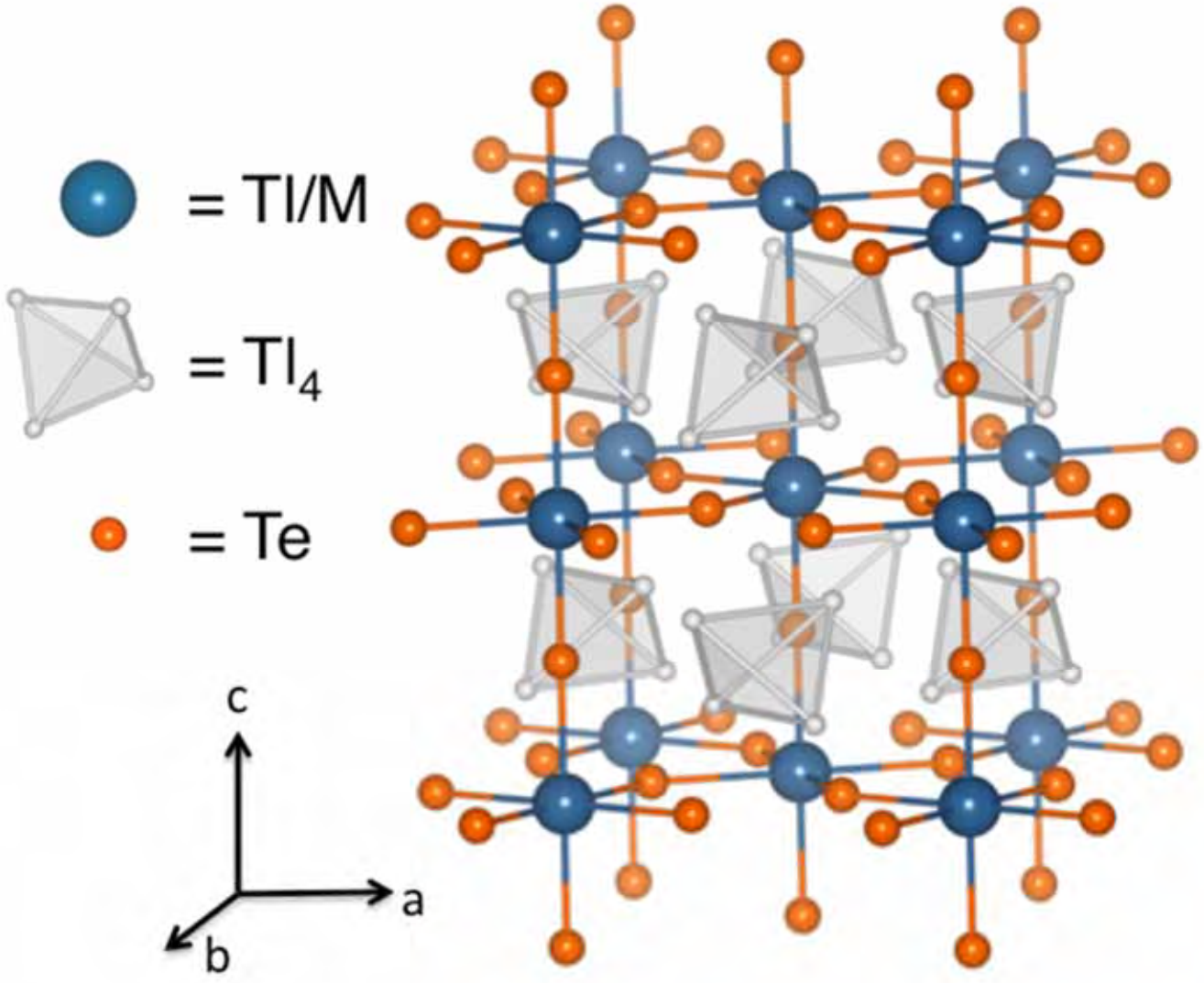
Superconductors with Dirac States?

TABLE 4 (Cont'd). Properties of Semiconductive Superconductive Materials

NOTE: "HF" Signifies high-magnetic-field data in Table 5.

Material	T_c(K)	H_o (oersted)	n	Crystal Structure	T_n(K)	Refs.
$P_{0.4}Sn_{0.6}$	1.24-1.10		2.2×10^{22}			930
$Pb_{0-0.12}Sn_{1-0.88}Te$	2.1-2.8-1.85		$1.1-1.6-0.1\times10^{20}$			1489
$Pb_{0.25-0.45}Sn_{0.75-0.55}Te$	0.064-0.012		$5.3-2.5\times10^{20}$			1674
PbTe			$10^{18}-10^{19}$, 5.0×10^{20}		0.009	770
$PtSb_2$			3.7×10^{20}		0.037	770
SbSn	1.60		2.9×10^{22}			1605
$Sb_{0.005-0.01}Sn_{0.07}Te_{0.995-0.99}$	0.022-0.068		$0.365-1.04\times10^{21}$			1605
SbTe			5.0×10^{20}	B1	0.051	770
SnTe	0.065-0.207		$1.05-2\times10^{21}$	B1		1605 770#
SnTe	0.01-0.214	HF	$0.3-2\times10^{21}$	B1		1605 1022 687
$Sn_{0.990-0.965}Te$	0.024-0.0168		$0.463-1.34\times10^{21}$	B1		1605 1566#
$Sn_{1-x}Te$	0.07-0.22		$1.05-2\times10^{21}$	B1		482 770#
	0.02-1.1		$0.4-7.5\times10^{21}$			
Te (P=40-70 kbar)	2.05		$1-4\times10^{18}$			
Te_3Tl_5	2.14, 2.19-2.23	HF	$>2\times10^{21}$	CUB		848

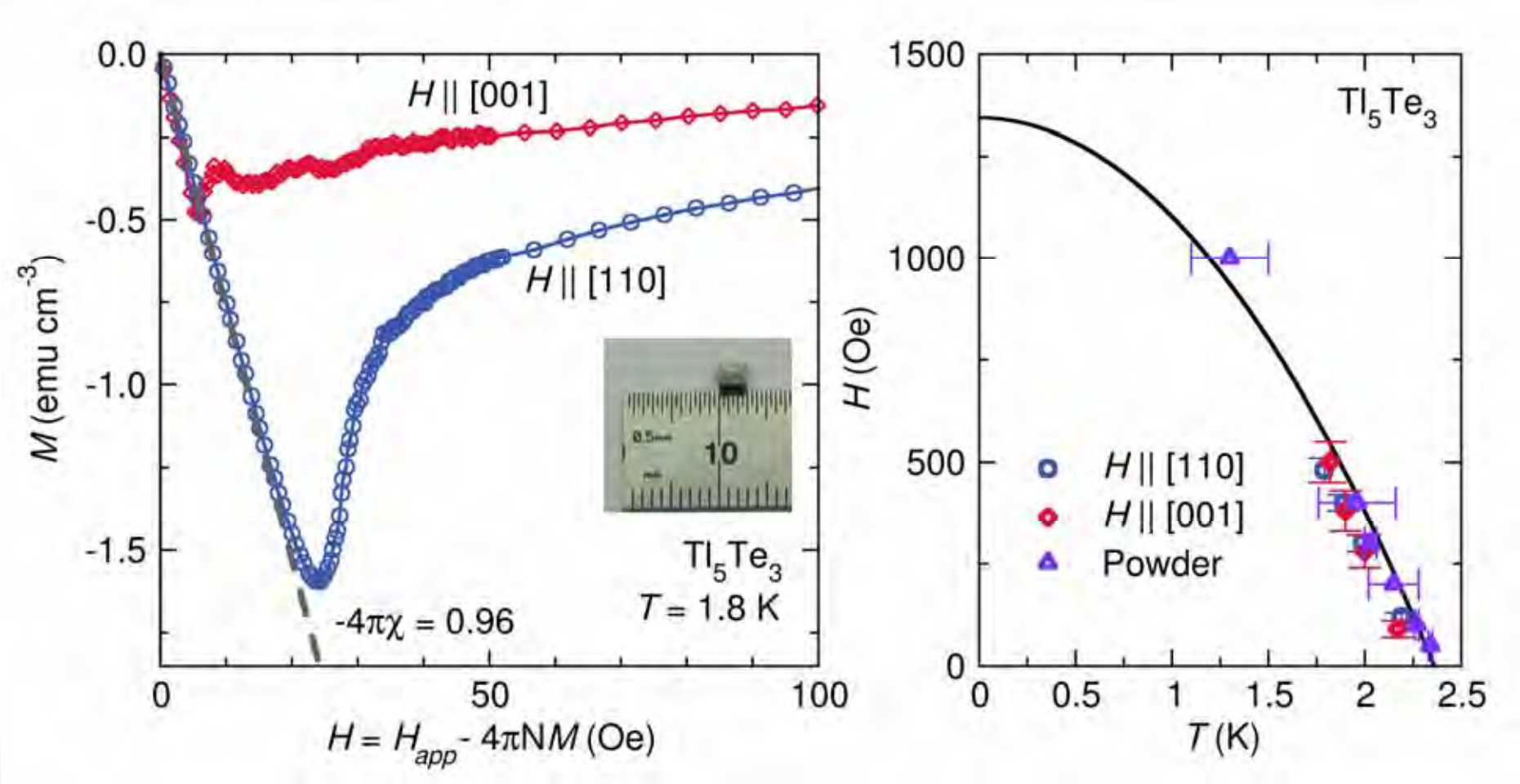
$[Tl_4]TlTe_3$: A Perovskite



Tl^{2+}: Negative U ion (U ~ -5 eV)

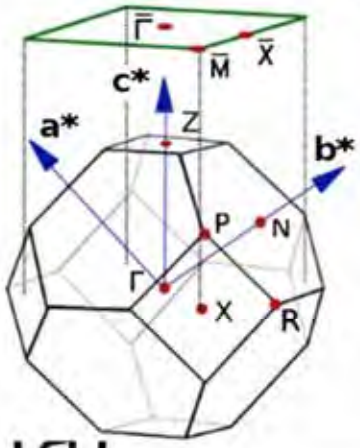
K.E. Arpino, et al. *Phys. Rev. Lett.* **112**, 017002 (2014)

Superconductivity ~ 2.5 K



K.E. Arpino, et al. *Phys. Rev. Lett.* **112**, 017002 (2014)

ARPES (hard!)



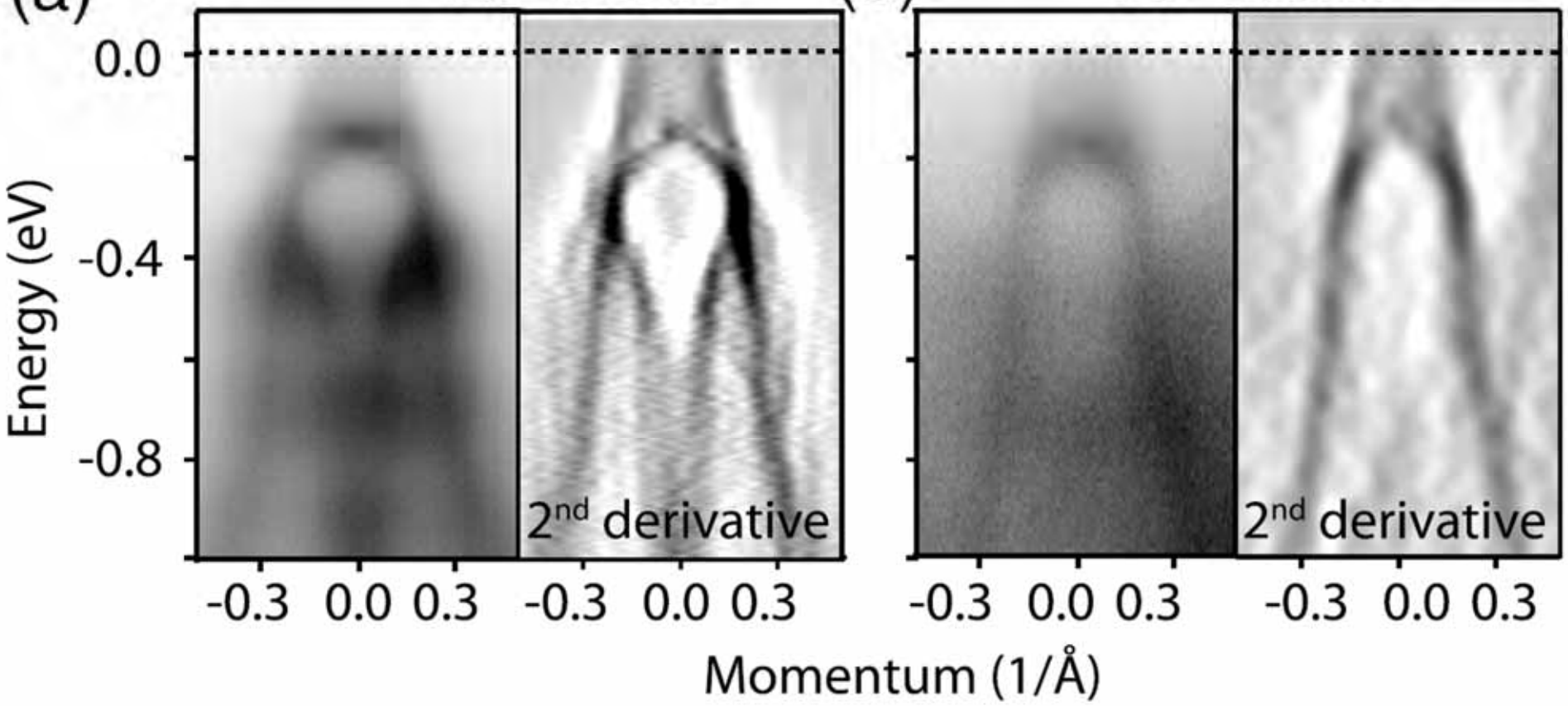
Tl_5Te_3

(a)

$h\upsilon = 21.2$ eV

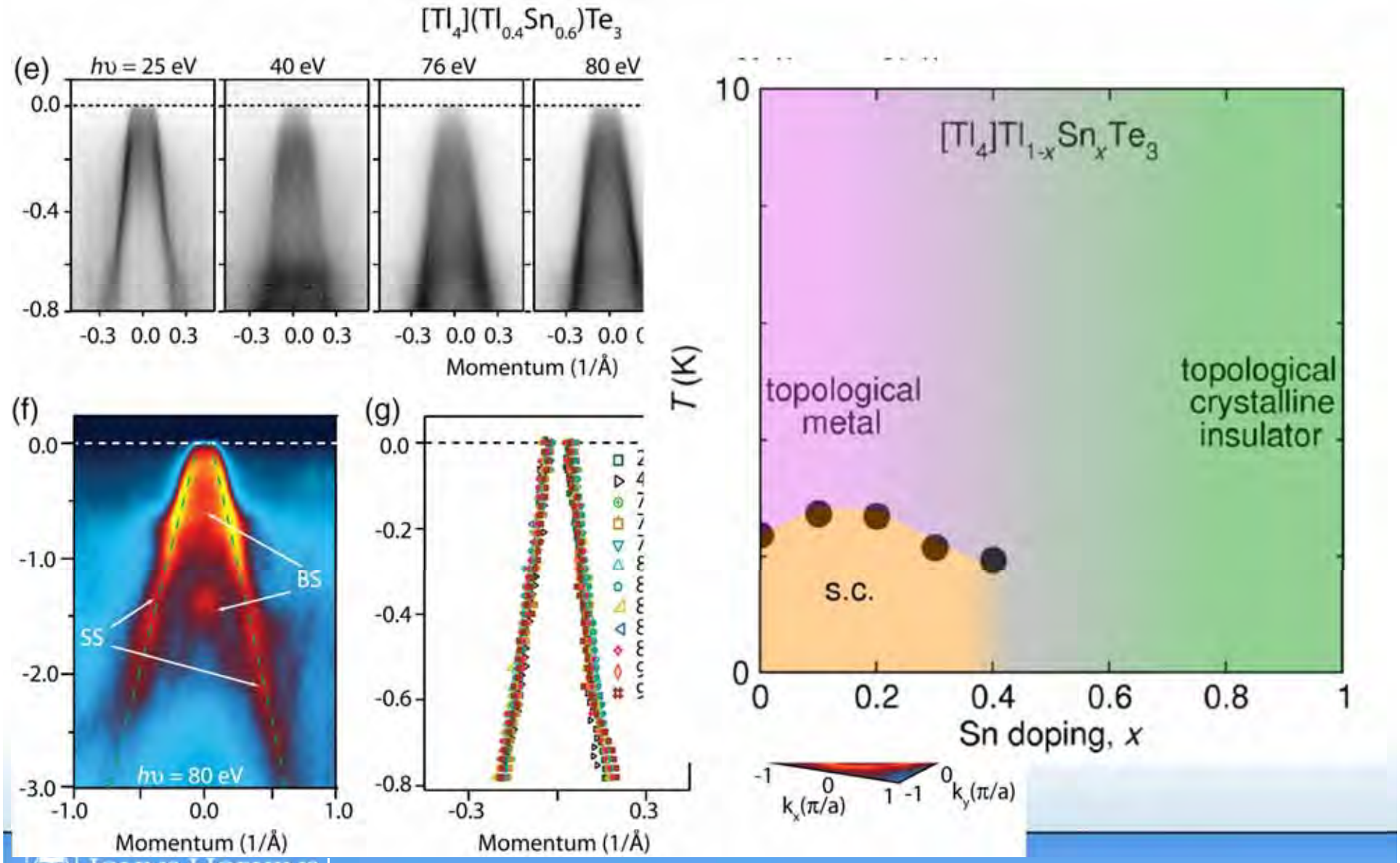
(b)

$h\upsilon = 40.8$ eV



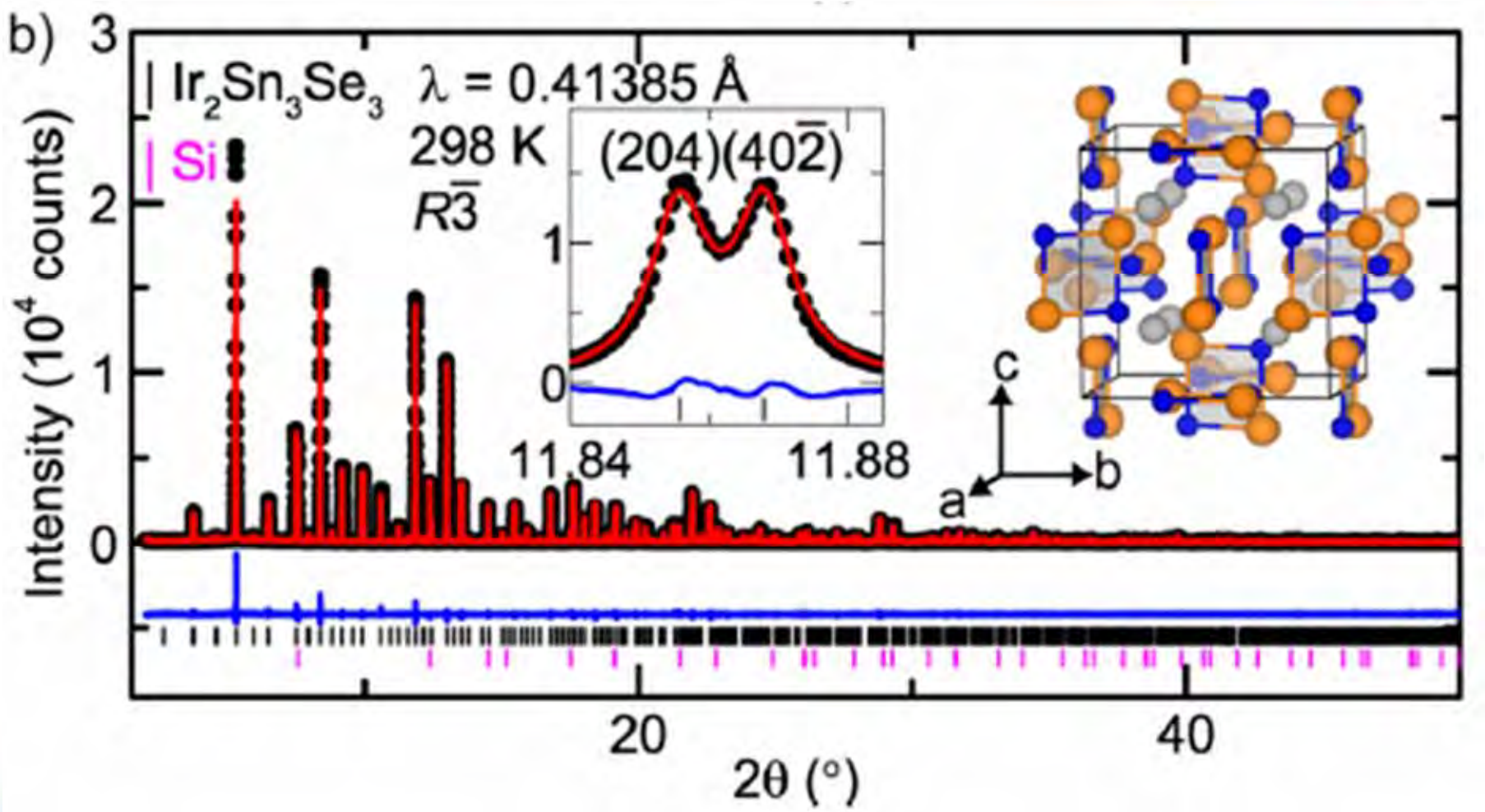
K.E. Arpino, et al. *Phys. Rev. Lett.* **112**, 017002 (2014)

$[Tl_4](Tl_{0.4}Sn_{0.6})Te_3$: Surface States Survive



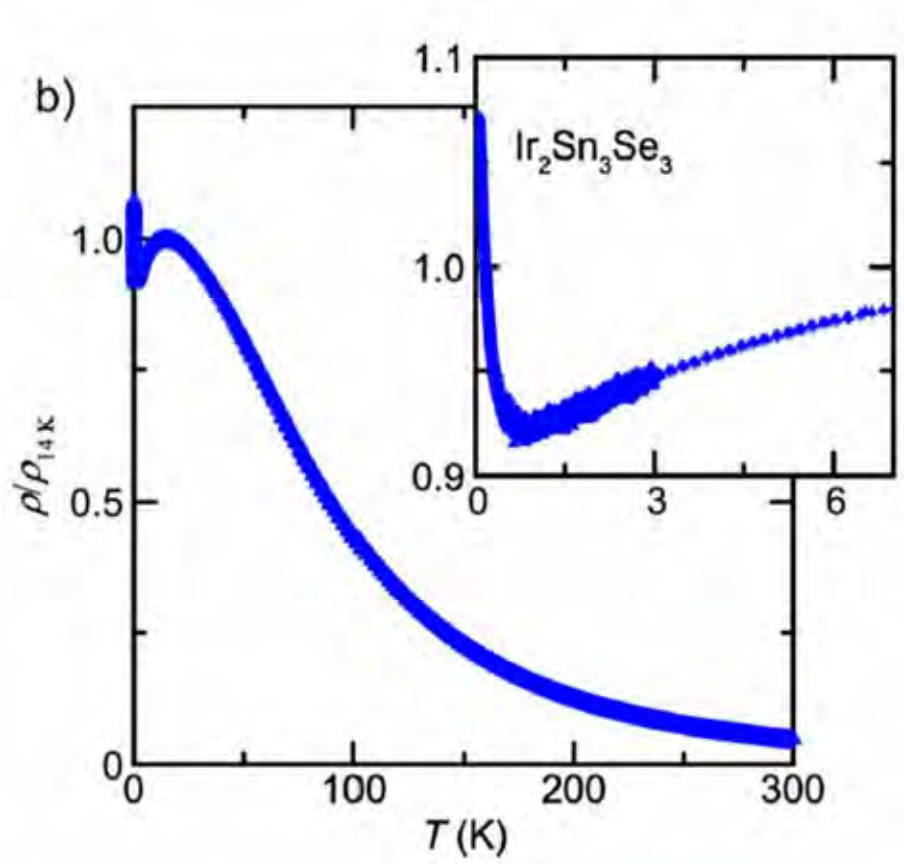
K.E. Arpino, et al. *Phys. Rev. Lett.* **112**, 017002 (2014) and *APL Mat.* **3**, 041507 (2015)

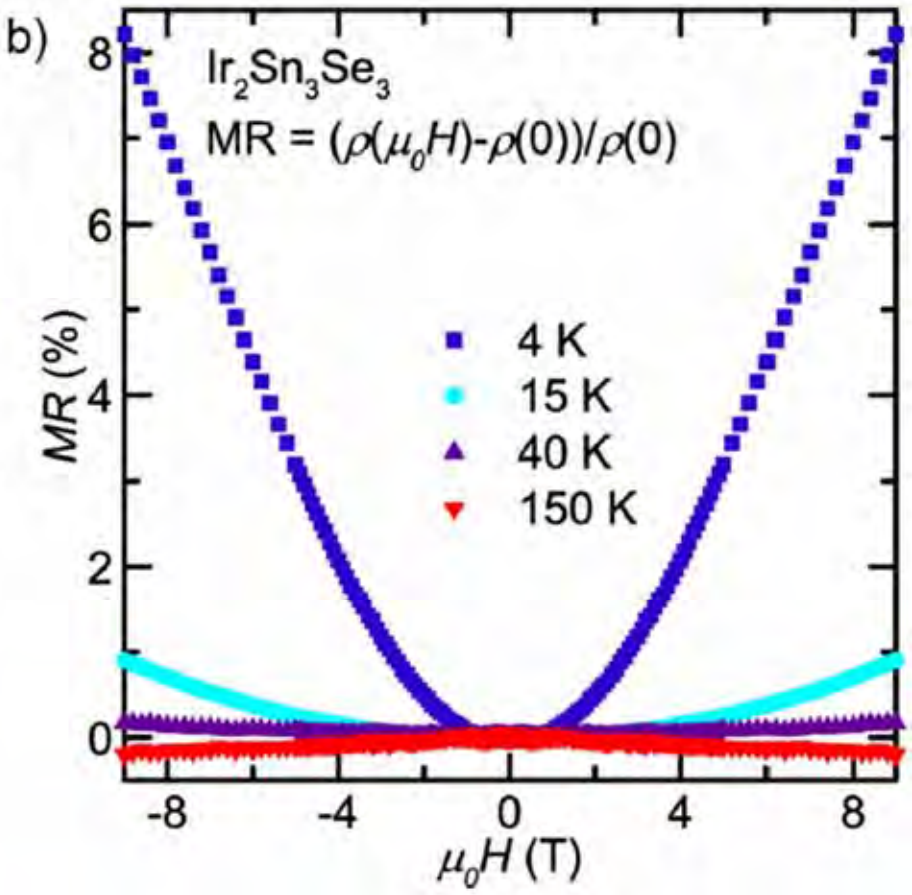
Iridium Skutterudites



B.A. Trump, et al. *Inorg. Chem.* 54, 11993-12001 (2015)

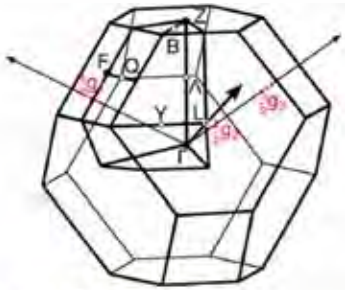
$Ir_2Sn_3Se_3$

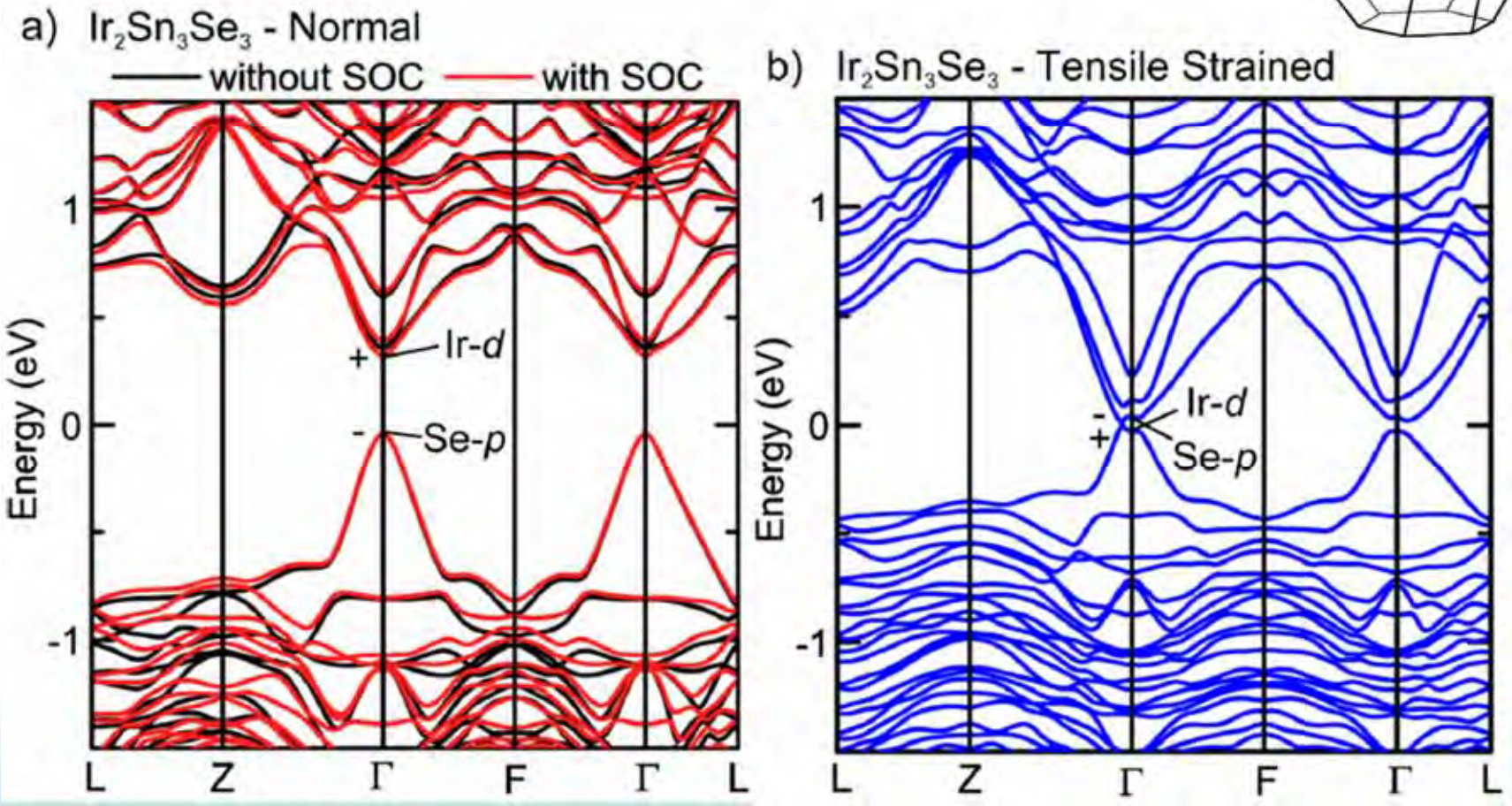




B.A. Trump, et al. *Inorg. Chem.* 54, 11993-12001 (2015)

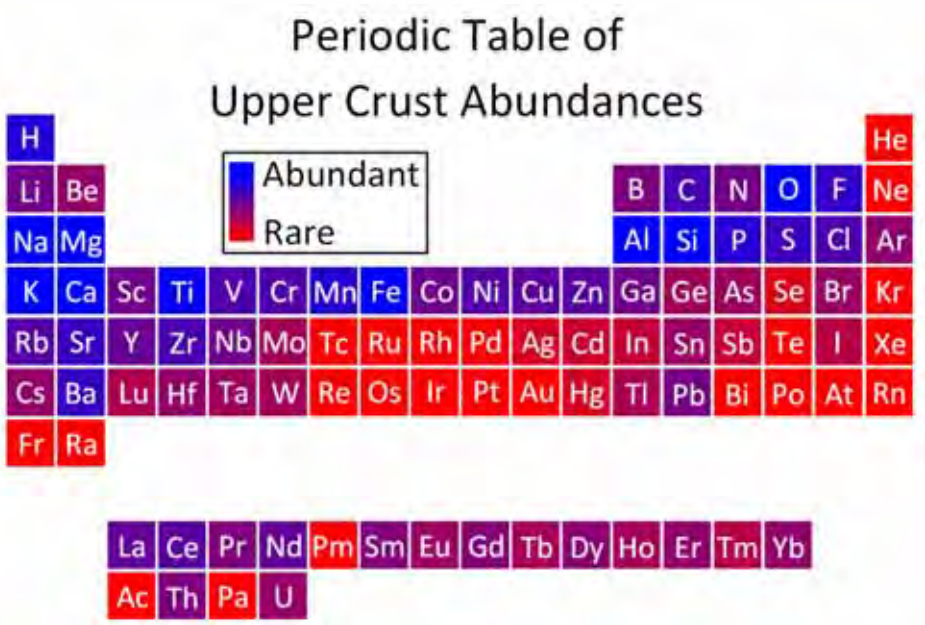
Topological Phase Transition When Strained?





B.A. Trump, et al. *Inorg. Chem.* **54**, 11993-12001 (2015)

Final Thoughts?



PRIOR ART

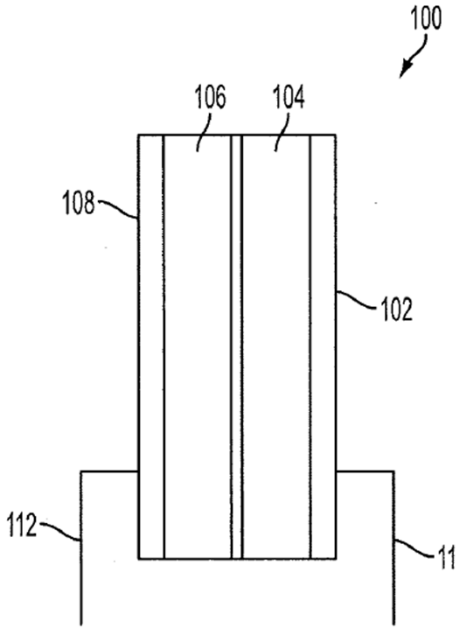


FIG. 1

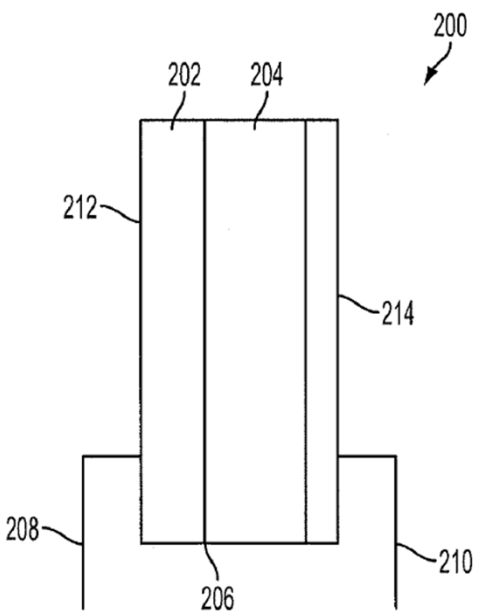


FIG. 2